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Zinc oxide is one of the uncommon optically transparent oxides which, doped, exhibits type-n conducting properties. Besides, ZnO is also expected to become a p-type transparent conductor under particular conditions. Although fascinating properties of such unusual material may lead to a new vast area of novel applications, there are several problems, which remain open at present. This unique predisposition is supposed to appear under some (and still unknown) modifications of the energy band structure, which impose to improve our knowledge on the electronic and structural properties of this material.

The well-known zinc oxide phase transition from B4 (hexagonal wurtzite structure) to B1 (rocksalt structure) has been studied by energy dispersive powder diffraction technique up to 11 GPa and 1273 K. Thermal equation of state of the cubic high-pressure ZnO phase has been determined for the first time. The previously (and apparently) well-demonstrated P-T phase diagram is shown to be incorrect. It is established that the B4-B1 transition is reversible and occurs with a dP/dT slope close to zero. These new results are confirmed by using simultaneously three other different types of experiment (x-ray imaging, ultrasonic and x-ray diffraction studies on single crystal).

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